L1 L2 L3	FILE	'REGISTRY' ENTERED AT 16:12:04 ON 22 OCT 2010 STRUCTURE UPLOADED 0 S L1 3 S L1 SSS FULL
L4	FILE	'HCAPLUS' ENTERED AT 16:12:49 ON 22 OCT 2010 3 S L3
L5 L6 L7	FILE	'REGISTRY' ENTERED AT 16:32:25 ON 22 OCT 2010 STRUCTURE UPLOADED 0 S L5 5 S L5 SSS FULL
L8	FILE	'HCAPLUS' ENTERED AT 16:33:34 ON 22 OCT 2010 4 S L7

=> file reg COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.22 0.22

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STRUCTURE FILE UPDATES: 21 OCT 2010 HIGHEST RN 1246809-78-8 DICTIONARY FILE UPDATES: 21 OCT 2010 HIGHEST RN 1246809-78-8

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

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http://www.cas.org/support/stngen/stndoc/properties.html

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Uploading C:\Program Files\STNEXP\Queries\10546132left.str

Chain nodes: 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 48 ring nodes: 1 2 3 4 5 6 chain bonds: 1 10 3-1 3-1 3-1 3-1 4 14-15

14-21 15-16 16-17 17-18 18-19 19-20 25-26 26-27 26-28 28-29 29-30 30-31 31-32 32-33 33-34 34-35 35-36 36-37 37-38 39-40 40-41 42-43 43-44

34-35 35-36 36-37 37-38 39-40 40-41 42-43 43ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6

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exact/norm bonds :
1 - 2 \quad 1 - 6 \quad 1 - 11 \quad 2 - 3 \quad 2 - 10 \quad 3 - 4 \quad 4 - 5 \quad 5 - 6 \quad 5 - 9 \quad 6 - 25 \quad 9 - 48 \quad 10 - 23 \quad 14 - 21 \quad 25 - 26
26-27
39-40
exact bonds :
3-7 7-8 8-24 11-12 12-13 13-14 14-15 15-16 16-17 17-18 18-19 19-20 26-28
28-29 29-30 30-31 31-32 32-33 33-34 34-35 35-36 36-37 37-38 40-41 42-43
43-44
G1:H,P
G2:H,[*1],[*2]
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS
21:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
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FULL FILE PROJECTIONS: ONLINE **COMPLETE**
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PROJECTED ITERATIONS:
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PROJECTED ANSWERS:
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
Structure attributes must be viewed using STN Express query preparation.
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100.0% PROCESSED 8843 ITERATIONS
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SEARCH TIME: 00.00.01
1.3
            3 SEA SSS FUL L1
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- L3 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN  $\alpha$ -D-Glucopyranose, 2-deoxy-3-0-[(3R)-3-methoxydecyl]-6-0-methyl-2-
- [[(112)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate)
  1-(2,2,2-trichloroethanimidate)
- MF C44 H78 C13 N2 O10 P

Absolute stereochemistry.

Double bond geometry as shown.

$$\begin{array}{c} \text{NH} \\ \text{C13C} \\ \text{Me} \end{array} \begin{array}{c} \text{C13C} \\ \text{OMe} \\ \text{OMe} \\ \text{OMe} \\ \text{R} \\ \text{R} \\ \text{R} \\ \text{OMe} \\ \text{OMe} \\ \text{H}_{2} \\ \text{OMe} \\ \text{H}_{2} \\ \text{OMe} \\ \text{$$

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

- L3 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- IN α-D-Glucopyranoside, (1Z)-1-propen-1-yl
- 2-deoxy-3-0-[(3R)-3-methoxydecyl]-6-0-methyl-2-[[(11Z)-1-oxo-11-octadecen-1-yl]amino]-
- MF C39 H73 N O7

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 5 
$$\underline{z}$$
 (CH<sub>2</sub>) 9  $\underbrace{R}_{R}$   $\underbrace{S}_{S}$  Me  $\underbrace{R}_{S}$   $\underbrace{R}_{S}$   $\underbrace{S}_{S}$   $\underbrace{N}_{S}$  OMe

L3 3 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN a-D-Glucopyranoside, (12)-1-propen-1-y1
2-deoxy-3-0-[(3R)-3-methoxydecy1]-6-0-methy1-2-[[(112)-1-oxo-11-octadecen-1-y1]mino]-, 4-(di-2-propen-1-y1) phosphate)

MF C45 H82 N O10 P

Absolute stereochemistry.
Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

#### ALL ANSWERS HAVE BEEN SCANNED

=> file hcaplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 191.54 191.76

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 16:12:49 ON 22 OCT 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 22 Oct 2010 VOL 153 ISS 18
FILE LAST UPDATED: 21 Oct 2010 (20101021/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2010

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13 L4 3 L3

=> d 14 1-3 ti abs bib hitstr

- L4 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
- TI Sodium salt of glucosamine disaccharide compound, method for producing the same, and use of the same
- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB There are disclosed a sodium salt represented by the average formula (I, m1, n1, m2 and n2 independently represent 0 or a pos. number not more than 2, while satisfying m1 + n1 = 2, m2 + n2 = 2, 0 < m1 + m2 < 4 and 0 < n1 + n2 < 4 .) and a method for producing such a sodium salt. There is also a decomposition suppressing method which enables to have a sodium salt represented by the average formula I coexistent with a sodium salt represented by the general formula II below. This method enables to improve long-term stability of a sodium salt represented by the general formula II which is effective for the prevention and/or treatment of septicemia caused by gram pos. bacteria, in particular endotoxin shock. Thus, a DEAE column main fraction containing 6.0 g disaccharide free acid (III) (preparation given) and
- 4.80 weight% Na and 942.8 L MeOH were stirred in a 4 L flask at 25°, treated with 0.2 N NaOH/MeOH solution (15.2 mL), stirred overnight, filtered, and treated dropwise with 270 mL acetone at 25°. The precipitate was removed by filtration and dried in vacuo to give III.3.67 Na. When III.3.67 Na was stored in a screw-cap bottle at 25° for 30 days, impurities A, B, and C were formed at a rate of 0.072, 0.267, and 0.072 %/mo, resp., vs. 0.729. 3.117, and 0.033 %/mo, resp., for III.4.06Na.
  AN 2008:636616 HCAPLUS <LOGINID: 220101022>>
- DN 149:10241
- TI Sodium salt of glucosamine disaccharide compound, method for producing the same, and use of the same
- IN Sakurai, Shin; Furukawa, Ken; Matsuo, Kimihiro; Tagami, Kenichi
- PA Eisai R & D Management Co., Ltd., Japan
- SO PCT Int. Appl., 46 pp. CODEN: PIXXD2

PATENT NO

- DT Patent
- LA Japanese FAN.CNT 1

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PI	WO 2008062842					A1		2008	0529		WO 2	007-	JP72	579		2	0071	121		
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KIND DATE APPLICATION NO DATE

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PRAI JP 2006-315020
                          Α
                                20061122
     US 2006-860483P
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     WO 2007-JP72579
                          W
                                20071121
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
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748165-18-6P 748165-20-0P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; preparation of sodium salt of glucosamine disaccharide

compound with storage stability, method for producing it, and its use for prevention and/or treatment of endotoxin shock)

RM 748165-18-6 HCAPLUS

α-D-Glucopyranoside, (1Z)-1-propen-1-yl

2-deoxy-3-0-[(3R)-3-methoxydecyl]-6-0-methyl-2-[[(11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RM 748165-20-0 HCAPLUS

CN [[(11Z)-1-oxo-11-octadecen-1-y1]amino]-, 4-(di-2-propen-1-y1 phosphate) 1-(2,2,2-trichloroethanimidate) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me 
$$(CH_2)_5$$
 Z  $(CH_2)_9$   $(CH_2)_6$   $(CH_$ 

IT 748165-17-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of sodium salt of glucosamine disaccharide compound with

storage

stability, method for producing it, and its use for prevention and/or treatment of endotoxin shock)

RN 748165-17-5 HCAPLUS

CN  $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl

2-deoxy-3-0-[(3R)-3-methoxydecy1]-6-0-methy1-2-[[(11Z)-1-oxo-11-octadecen-1-y1]amino]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

Me (CH<sub>2</sub>) 
$$\frac{z}{z}$$
 (CH<sub>2</sub>)  $\frac{z}{z}$  (CH<sub>2</sub>)  $\frac{z}{z}$  Me Ne OH

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
- TI Process for production of lipid A analogue GI

AR There is disclosed a process for producing

3-0-decy1-2-deoxy-6-0-[2-deoxy-3-0-[(3R)-3-methoxydecy1]-6-0-methy1-2-[(112)-1-oxo-11-octadecenyl]amino $]-4-O-phosphono-\beta-D-glucopyranosyl]-$ 2-[(1,3-dioxotetradecyl)amino]-α-D-glucopyranose 1-(dihydrogen phosphate) (known as eritoran) tetrasodium salt (I; R = PO3Na2) which is useful as an active ingredient of a pharmaceutical or an intermediate for the synthesis thereof. A process for producing the compound I (R = PO3Na2) comprises the key steps of reacting a compound represented by the formula I [R = P(O)(OCH2CH:CH2)2] with a palladium catalyst in the presence of a nucleophilic agent (deallylation) and treating the product with a sodium source (sodium salt formation). This process is environment-friendly and excellent in safety, operationability, and reproducibility. Thus, a solution of 101.6 g I [R = P(O)(OCH2CH:CH2)2] in 203 mL THF was added to a mixture of Meldrum's acid 70.49, palladium acetate 2.93, and PPh3 51.3 g and the resulting mixture was stirred at 32° for 2 h and at 30° for 4 h, treated with 250 mL MeOH, and concentrated under reduced pressure to give a

residue (466.7 g). The residue was dissolved in 4,570 mL MeOH at 40°, treated with 5.55 g trimercaptotriazine, stirred overnight at

room temperature, and filtered to remove the precipitated

trimercaptotriazine-palladium

complex, followed by washing the precipitate with MeOH to give a combined filtrate (4,330 g). The filtrate (3,908.2 mL) was concentrated under reduced pressure to give a residue (440.9 g) which was treated with 450 mL acetone, concentrated under reduced pressure, treated again with 450 mL

acetone, and concentrated under reduced pressure. The residue was refrigerated overnight, treated with 1,800 mL acetone, warmed to 40°, stirred

for 1.5 h, air-cooled, stirred at ≥30° for 1.5 h, and filtered to give, after washing with acetone and drying at 35-40°

under reduced pressure, 74.2% eritoran (free acid form) which was treated with 0.1 N aqueous NaOH solution to give eritoran tetrasodium salt.

2007:257680 HCAPLUS <<LOGINID::20101022>>

AN DN 146:317153

Process for production of lipid A analogue

Tagami, Katsuya; Sato, Keizo; Matsuo, Kimihiro; Abe, Taichi; Haga, IN Tovokazu

PA Eisai R & D Management Co., Ltd., Japan

SO PCT Int. Appl., 69pp. CODEN: PIXXD2

Pat.ent.

LA Japanese

FAN	.CNT	1	

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PΙ	WO 2007026675	A1	20070308	WO 2006-JP316941	20060829

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     WO 2006-JP316941
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                                20060829
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
     CASREACT 146:317153
     748165-18-6P
                    748165-20-0P
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
     preparation); PREP (Preparation); RACT (Reactant or reagent)
        (process for production of lipid A analog (eritoran) via
        palladium-catalyzed deallylation of eritoran diallyl ester and
        formation of sodium salt)
```

2-deoxy-3-0-[(3R)-3-methoxydecy1]-6-0-methy1-2-[[(11Z)-1-oxo-11-octadecen-

1-y1]amino]-, 4-(di-2-propen-1-y1 phosphate) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

748165-18-6 HCAPLUS

RN

RN

Me (CH<sub>2</sub>) 5 
$$\overline{Z}$$
 (CH<sub>2</sub>) 9  $\overline{R}$   $\overline{R}$ 

 $\alpha$ -D-Glucopyranoside, (1Z)-1-propen-1-yl

748165-20-0 HCAPLUS  $\alpha$ -D-Glucopyranose, 2-deoxy-3-0-[(3R)-3-methoxydecyl]-6-0-methyl-2-CN [[(11Z)-1-oxo-11-octadecen-1-y1]amino]-, 4-(di-2-propen-1-y1 phosphate)

#### 1-(2,2,2-trichloroethanimidate) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

TT 748165-17-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(process for production of lipid A analog (eritoran) via
palladium-catalyzed deallylation of eritoran diallyl ester and
formation of sodium salt)

RN 748165-17-5 HCAPLUS

CN α-D-Glucopyranoside, (1Z)-1-propen-1-yl

2-deoxy-3-0-[(3R)-3-methoxydecyl]-6-0-methyl-2-[[(11Z)-1-oxo-11-octadecen-1-yl]amino]- (CA INDEX NAME)

#### Absolute stereochemistry.

Double bond geometry as shown.

# RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2010 ACS on STN
- TI Reagents and methods for preparing lipopolysaccharides antagonist B1287 and stereoisomers thereof for treatment of various forms of septic shock

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- The present invention provides methods for preparing lipopolysaccharides (LPS) antagonist lipo-disaccharide B1287 and stereoisomers thereof, which compds. are useful as in the prophylactic and affirmative treatment of endotoxemia including sepsis, septicemia and various forms of septic shock (no biol. data). Also provided are synthetic intermediates useful for implementing the inventive methods. Thus, lipo-disaccharide B1287 I was prepared for treatment of various forms of septic shock.
- AN 2004:718552 HCAPLUS <<LOGINID::20101022>>
- DN 141:225771 ΤI Reagents and methods for preparing lipopolysaccharides antagonist B1287
  - and stereoisomers thereof for treatment of various forms of septic shock
- TN Fan, Rulin
- PA Eisai Co, Ltd., Japan
- so PCT Int. Appl., 175 pp. CODEN: PIXXD2
- DT Patent.
- LA English

FAN.	CNT	1																
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PRAI	US	2003	-448	839P		P		2003	0220									
	WO	2004	-US4	921		W		2004	0218									

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

- CASREACT 141:225771; MARPAT 141:225771
- ΙT 748165-17-5P 748165-18-6P 748165-20-0P
  - RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reagents and methods for preparing lipopolysaccharides antagonist b and stereoisomers thereof for treatment of various forms of septic shock) 748165-17-5 HCAPLUS

- RN CN  $\alpha$ -D-Glucopyranoside, (12)-1-propen-1-yl
  - 2-deoxy-3-0-[(3R)-3-methoxydecy1]-6-0-methy1-2-[[(11Z)-1-oxo-11-octadecen-1-vllaminol- (CA INDEX NAME)

RN 748165-18-6 HCAPLUS
CN α-D-Glucopyranoside, (1Z)-1-propen-1-y1
2-decyu-3-0-(13P)-3-methovydecyul-6-0-methy

2-deoxy-3-0-[(3R)-3-methoxydecyl]-6-0-methyl-2-[[(11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 748165-20-0 HCAPLUS

CN  $\alpha$ -D-Glucopyranose, 2-deoxy-3-0-[(3R)-3-methoxydecyl]-6-0-methyl-2-[(11Z)-1-oxo-11-octadecen-1-yl]amino]-, 4-(di-2-propen-1-yl phosphate) 1-(2,2,2-trichloroethanimidate) (CA INDEX NAME)

OSC.G 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 16:11:50 ON 22 OCT 2010)

FILE 'REGISTRY' ENTERED AT 16:12:04 ON 22 OCT 2010

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 3 S L1 SSS FULL

FILE 'HCAPLUS' ENTERED AT 16:12:49 ON 22 OCT 2010 L4 3 S L3

=> log hold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 20.34 212.10 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -2.55-2.55

SESSION WILL BE HELD FOR 120 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 16:13:03 ON 22 OCT 2010

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:SSPTAEX01623

PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* \*
SESSION RESUMED IN FILE 'HCAPLUS' AT 16:32:18 ON 22 OCT 2010

## FILE 'HCAPLUS' ENTERED AT 16:32:18 ON 22 OCT 2010 COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL
FULL ESTIMATED COST	20.34	212.10
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.55	-2.55
=> file reg COST IN U.S. DOLLARS	SINCE FILE	TOTAL
CODI IN C.D. BOLLAND	ENTRY	SESSION
FULL ESTIMATED COST	20.34	212.10
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.55	-2.55

FILE 'REGISTRY' ENTERED AT 16:32:25 ON 22 OCT 2010
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 OCT 2010 HIGHEST RN 1246809-78-8
DICTIONARY FILE UPDATES: 21 OCT 2010 HIGHEST RN 1246809-78-8

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

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http://www.cas.org/support/stngen/stndoc/properties.html

= 3

Uploading C:\Program Files\STNEXP\Queries\10546132right.str

55 56 57 58 59 60 61 62 63 64 73 75 76 77 78 79 80 81 82 83 84 85 86 87 94 ring nodes : 1 2 3 4 5 6 40 41 42 43 44 45 65 66 67 68 69 70 71 72 74 91 chain bonds : 29-30 30-31 31-32 32-33 33-34 34-35 36-37 37-38 40-50 41-49 42-46 44-48 46-47 47-61 48-62 49-60 50-51 51-52 52-53 53-54 54-55 55-56 56-57 57-58 58-59 62-63 63-64 65-75 69-73 73-85 75-76 76-77 77-78 78-79 79-80 80-81 81-82 82-83 83-84 85-86 86-87

chain nodes :

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ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 40-41 40-45 41-42 42-43 43-44 44-45 65-66 65-70 66-67 66-67 674 67-8 67-71 68-69 69-70 71-72 72-91 74-91 exact/norm bonds:
1-2 1-6 1-11 2-3 2-10 3-4 4-5 5-6 5-9 9-36 23-24 23-94 24-25 27-39 40-41 40-45 40-50 41-42 41-49 42-43 43-44 44-45 44-48 48-62 65-66 65-70 65-75 66-7 66-76 67-74 67-68 67-71 68-69 69-70 69-73 71-72 72-91 73-85 74-91 exact bonds:
3-7 7-8 8-22 10-21 11-12 12-13 13-14 14-15 15-16 16-17 17-18 18-19 19-20 24-26 26-72 27-28 28-29 29-30 30-31 31-32 32-33 33-34 34-35 36-37 37-38 42-46 46-47 47-61 49-60 50-51 51-52 52-53 53-54 54-55 55-56 56-57 57-58 58-59 62-63 63-64 75-76 77-78 78-79 79-80 80-81 81-82 82-83 83-84 85-86 86-87
```

#### G1:[\*1],[\*2],[\*3]

```
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS
29:CLASS 30:CLASS
31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS
39:CLASS 40:Atom
41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:CLASS 47:CLASS 48:CLASS 49:CLASS
50:CLASS
51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS
59:CLASS 60:CLASS
61:CLASS 62:CLASS 63:CLASS 64:CLASS 65:Atom 66:Atom 67:Atom 68:Atom 69:Atom
70:Atom 71:Atom
72:Atom 73:CLASS 74:Atom 75:CLASS 76:CLASS 77:CLASS 78:CLASS 79:CLASS
80:CLASS 81:CLASS
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82:CLASS 83:CLASS 84:CLASS 85:CLASS 86:CLASS 87:CLASS 91:Atom 94:CLASS

### L5 STRUCTURE UPLOADED

=> s 15 SAMPLE SEARCH INITIATED 16:32:51 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 591 TO ITERATE

100.0% PROCESSED 591 ITERATIONS SEARCH TIME: 00.00.01 0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 1362 TO 13278
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 sss full FULL SEARCH INITIATED 16:33:18 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 12449 TO ITERATE

100.0% PROCESSED 12449 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

L7 5 SEA SSS FUL L5

=> d 17 scan

L7 5 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN β-D-Glucopyranoside, (1E)-1-propen-1-yl 3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-dioxotetradecyl)aminol-

MF C39 H75 N O7 Si

Absolute stereochemistry.
Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L7 5 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C36 H65 N O7

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 5 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN

N a-D-Glucopyranoside, (1Z)-1-propen-1-yl 3-0-decyl-2-deoxy-6-0-[(1.-dimethylethyl)dimethylsilyl]-2-[(1,3-dioxotetradecyl)amino]-

MF C39 H75 N O7 Si

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7 5 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN
- INDEX NAME NOT YET ASSIGNED IN
- C36 H65 N O7 MF

Absolute stereochemistry. Double bond geometry as shown.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- L7
- IN
- 5 ANSWERS REGISTRY COPYRIGHT 2010 ACS on STN  $\alpha\text{-D-Glucopyranoside,} \quad (1\text{Z})\text{-1-propen-1-y1} \\ 3\text{-O-decy1-2-deoxy-2-[(1,3\text{-dioxotetradecy1)amino]-}}$ C33 H61 N O7 MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

### => 0

0 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> file hcaplus COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	192.03	404.13
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL
CA SUBSCRIBER PRICE	0.00	-2.55

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FILE COVERS 1907 - 22 Oct 2010 VOL 153 ISS 18
FILE LAST UPDATED: 21 Oct 2010 (20101021/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2010

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 18 1-4 ti abs bib hitstr

L8 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2010 ACS on STN

TI Preparation of glucose lipid A analogs inhibiting macrophage activity

AB Title compds. I [Q = -O-, alkylene, -O-alkylene, etc.; W = -O- or -NH-; when W is -NH-, Rl is alkanoyl, alkenoyl, alkynoyl. (wherein alkanoyl, alkenoyl and alkynoyl are optionally substituted with halo, hydroxy, oxo, etc.); each Rl (when W is -O-), R2, R3, and R4 is H, alkyl, alkenyl, etc. (wherein alkyl and alkenyl are optionally substituted with halo, hydroxy, oxo, etc.); R5 = H, halo, hydroxy, etc.] and their pharmacol. acceptable salts were prepared For example, phosphono 3-O-decyl-2-deoxy-6-O-[3-O-[(R)-3-methoxydecyl]-6-O-methyl-2-O-[(Z)-11-octadecenoyl]-4-O-phosphono-β-D-glucopyranosyl]-2-(3-oxotetradecanoylamino)-α-D-glucopyranoside (II) was prepared from 1,2:5,6-di-O-isopropylidene-α-D-glucofuranose in 18 steps. In human TNFα production inhibition assays, the IC50 value of compound II was 0.49 nM. Compds. I are claimed useful for the treatment of inflammation.

Ι

autoimmune diseases, etc.
AN 2007:167289 HCAPLUS <<LOGINID::20101022>>

DN 146:252059

TI Preparation of glucose lipid A analogs inhibiting macrophage activity

IN Shiozaki, Masao; Shimozato, Rvuichi

PA Sankyo Co., Ltd., Japan

SO Jpn. Kokai Tokkvo Koho, 86pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1														
PA	TENT NO.	KIND	DATE	APPLICATION NO.	DATE									
PI JP	2007039450	A	20070215	JP 2006-187298	20060707									
PRAI JE	2005-199518	A	20050708											

OS MARPAT 146:252059

IT 859508-28-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of glucose lipid analogs for treatment of inflammation and

#### autoimmune diseases)

RN 859508-28-4 HCAPLUS

CN  $\beta$ -D-Glucopyranoside, (1E)-1-propen-1-yl

3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-dioxotetradecyl)amino]- (CA INDEX NAME)

- L8 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2010 ACS on STN
- TI Syntheses of glucose-containing E5564 analogs and their LPS-antagonistic activities
- AB Lipid A analogs containing a glucose moiety on their non-reducing end were synthesized, and their LPS-antagonistic activities were measured. The inhibitory activities (ICSO) on LPS-induced TNPA production of title aminodeoxy disaccharides toward human whole blood cells were 0.46-1.11 nM. Inhibitory doses (IDSO) of these compds. on TNPA production induced by co-injection of galactosamine and LPS in C3H/HeN mice were measured. The IDSO values of these compds. were 0.20-1.08 and <0.2 mg/kg. Moreover, C3H/HeN mice preinjected with compds. were protected from lethality induced by co-injection of galactosamine and LPS. Out of eight mice preinjected with 1 mg/kg of title compds. five-eight mice were protected.
- AN 2005:1299295 HCAPLUS <<LOGINID::20101022>>
- DN 144:171174
- TI Syntheses of glucose-containing E5564 analogs and their LPS-antagonistic activities
- AU Shiozaki, Masao; Doi, Hiromi; Tanaka, Daisuke; Shimozato, Takaichi; Kurakata, Shin-ichi
- CS Chemistry Department, Chemtech Labo, Inc., Hiromachi 1-2-58, Shinagawa-ku, Tokyo, 140-8710, Japan
- SO Tetrahedron (2005), Volume Date 2006, 62(1), 205-225 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier B.V.
- DT Journal
- LA English
- OS CASREACT 144:171174
- T 859508-28-4P
- RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
  - (syntheses of glucose-containing E5564 analogs and their LPS-antagonistic activities)
- RN 859508-28-4 HCAPLUS
- CN  $\beta$ -D-Glucopyranoside, (1E)-1-propen-1-y1
  - 3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-dioxotetradecyl)amino]- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

OSC.G 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2010 ACS on STN TI preparation of levulose glucoselipid A derivatives as  $\text{TNF}\alpha$  production inhibitors

AB Title compds. I [Q = O, etc.; W = O, NH; R1 = (un)substituted alkanoyl, etc. with the proviso that if W = NH; R1 (with the proviso that if W = O), R2, R3, R4 = H, (un)sunstituted alkyl, etc.; R5 = H, halo, etc.] were prepared For example, phosphorylation of 4-0-(allyloxycarbonyl)-3-0-decyl-2-deoxy-6-0-[4-0-diallylphosphono-3-0-[(R)-3-methoxydecyl]-6-0-methyl-2-0-[(Z)-11-octadecenoyl]- $\beta$ -Dqlucopyranosy1]-2-(3-oxotetradecanoylamino)-α-D-glucopyranoside, e.g., prepared from 1,2:5,6-di-O-isopropylidene-α-D-glucofuranose in 15 steps, with diallyl diisopropylphosphoramidate followed by deallylation using Pd(PPh3)4 afforded phosphono 3-0-decv1-2-deoxy-6-0-[3-0-[(R)-3-methoxydecv1]-6-0-methy1-2-0-[(Z)-11octadecenoy1]-4-0-phosphono-β-D-glucopyranosy1]-2-(3oxotetradecanoylamino)- $\alpha$ -D-glucopyranoside (II). In TNF $\alpha$ production inhibition assays, the IC50 value of compound II was 0.49 nM. Compds. I are claimed useful for the treatment of inflammation, septicemia, etc.

Ι

AN 2005:638895 HCAPLUS <<LOGINID::20101022>>

DN 143:153644

GI

TI preparation of levulose glucoselipid A derivatives as TNFα

```
production inhibitors
```

IN Shiozaki, Masao; Shimozato, Takaichi

PA Sankyo Company, Limited, Japan

SO PCT Int. Appl., 156 pp.

CODEN: PIXXD2

DT Patent LA Japanese

FAN.CNT 1

PAN.			мо.			KIND DATE					ICAT							
PI	WO	2005	0661	93				2005	0721								0050	107
		W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
												EC,						
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		1702		30				20050818 JP 2005-2028 20060920 EP 2005-703673										
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	CNI	1930				A						005-					1050	107
		2005										005-						
		2006										006-					0060	
		2006				A			0926			006-						
		2006										006-						
		2009							0305			008-					080	
PRAI		2004				A		2004								-		
		2005				W		2005										

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OS MARPAT 143:153644 IT 859508-28-4P

RL: RCT (Reactant); SFN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of levulose glucoselipid A derivs. as  ${\tt TNF}\alpha$  production inhibitors for treatment of inflammation, septicemia, etc.)

RN 859508-28-4 HCAPLUS

CN β-D-Glucopyranoside, (1E)-1-propen-1-yl

3-O-decyl-2-deoxy-6-O-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-dioxotetradecyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

#### RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L8 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2010 ACS on STN
- ΤI Reagents and methods for preparing lipopolysaccharides antagonist B1287 and stereoisomers thereof for treatment of various forms of septic shock
- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB The present invention provides methods for preparing lipopolysaccharides (LPS) antagonist lipo-disaccharide B1287 and stereoisomers thereof, which compds. are useful as in the prophylactic and affirmative treatment of endotoxemia including sepsis, septicemia and various forms of septic shock (no biol. data). Also provided are synthetic intermediates useful for implementing the inventive methods. Thus, lipo-disaccharide B1287 I was prepared for treatment of various forms of septic shock.
- 2004:718552 HCAPLUS <<LOGINID::20101022>> AN
- DM 141:225771
- ΤI Reagents and methods for preparing lipopolysaccharides antagonist B1287 and stereoisomers thereof for treatment of various forms of septic shock IN Fan, Rulin
- PA Eisai Co, Ltd., Japan
- PCT Int. Appl., 175 pp. SO
- CODEN: PIXXD2 DT Patent
- LA English
- EAN ONE

PAN.	WO 2004074303 W: AE, AG, A CN, CO, C GE, GH, G LK, LR, L RW: BW, GH, G BG, CH, C MC, NL, P GQ, GW, M JP 2006518394 US 20060160999					KIND DATE				APPL	ICAT		DATE					
PI						A2 A3		2004			WO 2	004-	US49	21		2	0040	218
			ΑE,	AG,		AM,		AU,	AZ,									
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,
			MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,								
	JP	2006			,	T		2006			JP 2	006-	5037	10		2	0040	218
	US	2006	0160	999		A1		2006	0720		US 2	005-	5461	32		2	0051	212
PRAI		2003				P		2003										
	WO	2004	-US4	921		W		2004	0218									

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT OS CASREACT 141:225771; MARPAT 141:225771

IT 748165-24-4P 748165-25-5P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (reagents and methods for preparing lipopolysaccharides antaqonist b and

stereoisomers thereof for treatment of various forms of septic shock)
748165-24-4 HCAPLUS

CN α-D-Glucopyranoside, (1Z)-1-propen-1-vl

3-0-decvl-2-deoxv-2-[(1,3-dioxotetradecvl)aminol- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 748165-25-5 HCAPLUS

CN α-D-Glucopyranoside, (12)-1-propen-1-y1 3-0-decy1-2-decyx-6-0-[(1,1-dimethylethyl)dimethylsilyl]-2-[(1,3-dioxotetradecyl)amino] (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

OSC.G 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT